# CFD Model setup:

## Boundary conditions

Precursor simulation was carried out with normal velocity of 53 m/s at the inlet [3], average static pressure = 0 Pa at outlet, outer wall defined as no slip wall, symmetry 1&2 defined as symmetry. The propane jet inflow conditions were provided by a precursor simulation of the fully developed pipe flow profile of the propane jet inlet pipe. The inflow conditions for the co-flow air inlet were also provided with an inlet flow profile, obtained from the experimental measurements. The fully developed flow profile for propane jet inlet included the flow variables velocity u, v, and w along with turbulence quantities k, ω and ε. For co-flow inlet the profile the flow quantities velocity u, v and w were provided. Turbulent inlet boundary conditions for co-flow inlet were taken, as Fractional Intensity = 5%, Eddy viscosity ratio = 10, as per mentioned in the literature [3]

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| --- | --- | --- |
| Boundary | ANSYS CFX | ANSYS Fluent |
| Co-flow inlet | Cartesian velocity components provided from Inlet profile  Turbulence Intensity = 5%  Eddy viscosity ratio = 10 | Cartesian velocity components provided from Inlet profile  Turbulence Intensity = 5%  Eddy viscosity ratio = 10 |
| Jet inlet | Cartesian velocity components along with turbulence inlet boundary condition provided from the fully developed flow profile | Cartesian velocity components along with turbulence inlet boundary condition provided from the fully developed flow profile |
| Bluff body | No slip wall | No slip wall |
| Symmetry 1 & 2 | Symmetry | Symmetry |
| Outer wall | Free slip wall | Free slip wall |
| Outlet | Avg. static pressure = 0 Pa | Gauge pressure = 0 Pa |

Table 5

## Material properties

Pure propane was used as fuel in the precursor simulation. Pure propane is injected in to the domain through the jet inlet and air at constant velocity flows through co-flow inlet. Here air is used as a mixture comprising of Ar (1.28 %), O2 (23.18%), N2 (75.53%), CO2 (0.0035%) of gas phase combustion material. For this investigation a mixture has been created with propane and above mentioned gases which constitute air, defined as a variable composition mixture. N2 is defined as a constraint [12]. Kinematic diffusivity has been defined same for all the species of mixture = 1.2045x10-5 m2/s obtained from [16].

Mass fraction of propane was defined as 1 and for others to be 0 at jet inlet.

## Initialization

Before starting the solver to compute, initialization of all the solution variables is a pre-requisite. A realistic initial guess improves solution stability and accelerates convergence. Poor initial guess may cause the solver to even fail during the first few iterations.

ANSYS CFX 16.1

In order to have the identical experimental conditions in the simulation it was decided to initially fill the domain with air. Global initialization [12] option was used. Velocity was specified in terms of all three components velocity u = 9.2 m/s, v and w = 0 m/s. Static pressure and turbulence boundary conditions were chosen to be of default solver value. The mass fractions of the species were only specified for all the gases which constitute air, except propane.

ANSYS Fluent 17.0

In fluent no such option as in CFX is available for initialization. Rather initialization was done using the option called hybrid initialization [13]. This is the default initialization method in Fluent which provides a quick approximation of the flow field, by a collection of methods.

## Numerical Settings

ANSYS CFX 16.1

The advection scheme and the turbulent numerics were chosen to be of High Resolution method [12]. Time scale for all the simulations was chosen to be Auto Timescale, which is the default option available in ANSYS CFX 16.1. Auto timescale control is a fluid timescale control option which uses an internally calculated physical time scale based on the boundary conditions, flow conditions, physics and domain geometry. The residual type MAX (maximum) with the target of 1e-05 was chosen as the convergence target and conservation target of 1e-03. The maximum number of iterations for all simulations was chosen to be 500.

ANSYS Fluent 17.0

Flow analysis chosen here is of steady state type with pressure-based [13] solver. In all simulations Coupled method [13] is chosen for the pressure-velocity coupling. The gradient approximation is done by Least Squares Cell Based method [13]. For pressure PRESTO [13] method has been used. For momentum second order upwind scheme is used. Turbulent numerics have been approximated by using the First order upwind scheme. For all the species transport again a second order upwind scheme is used. Pseudo transient and higher order term relaxation [13] has also been selected. The residual type RMS (Root mean square) with a target of 1e-07 is selected for each solution variable. Time step method was chosen to be automatic with 500 as the maximum number of iterations for all the simulations

## Post-Processing

Post-processing of the results have been carried in ANSYS CFD Post 16.1 using the pearl scripts and gnuplot scripts for plotting the data extracted from CFD Post for comparison with the experimental data.